# CLAIMS

We claim:

1. A method for analyzing multivariate images, comprising:

a) providing a data matrix **D** containing measured spectral data,

b) reading an $i^{th}$ block of data $\mathbf{D}_i$ of a total of $j$ data blocks from the data matrix **D** into the memory of a computer,

c) computing a block crossproduct matrix $\mathbf{D}_i^T\mathbf{D}_i$ from the data block $\mathbf{D}_i$,

d) adding the block crossproduct matrix $\mathbf{D}_i^T\mathbf{D}_i$ to an accumulation of the block crossproduct matrices,

e) repeating steps b) through d) until all $j$ of the data blocks $\mathbf{D}_i$ of the data matrix **D** are read, providing a crossproduct matrix $\mathbf{D}^T\mathbf{D}$,

f) performing an eigenanalysis of the crossproduct matrix to obtain eigenvectors **V** and eigenvalues **E**,

g) computing a loadings matrix **P**, according to **P** = **V**,

h) computing a scores matrix **T**, according to **T** = **DP**, and

i) performing an image analysis of $\mathbf{TP}^T$ to obtain a concentration matrix **C** and a spectral shapes matrix **S**.

2. The method of Claim 1, wherein the data block $\mathbf{D}_i$ is suitably sized to fit in the memory and consists of the full spectral data at some number of spectral channels.

3. The method of Claim 1, wherein $j = 1$.

4. The method of Claim 1, further comprising computing a weighted crossproduct matrix at step e) and using the weighted crossproduct matrix to perform the eigenanalysis in step f).

5. The method of Claim 1, further comprising computing a covariance matrix at step e) and using the covariance matrix to perform the eigenanalysis in step f).

6. The method of Claim 1, further comprising computing a correlation matrix at step e) and using the correlation matrix to perform the eigenanalysis in step f).

7. The method of Claim 1, wherein step g) further comprises retaining only the first $r$ columns of **V** so that **P** comprises the first $r$ significant eigenvectors of the eigenanalysis.

8. The method of Claim 1, wherein the image analysis comprises an alternating least squares analysis and the concentration matrix **C** and the spectral shapes matrix **S** are obtained from a constrained least squares solution to $\min_{\mathbf{C},\mathbf{S}} \left\| \mathbf{T}\,\mathbf{P}^{\mathrm{T}} - \mathbf{C}\mathbf{S}^{\mathrm{T}} \right\|_{\mathbf{F}}$.

9. The method of Claim 8, wherein the alternating least squares analysis comprises a non-negativity constraint.

10. The method of Claim 1, further comprising applying a wavelet transformation to the data block $\mathbf{D}_i$ after step b), to provide a transformed data block $\tilde{\mathbf{D}}_i$, and using the transformed data block to compute the block crossproduct matrix in step c), to provide a transformed concentration matrix $\tilde{\mathbf{C}}$ at step i).

11. The method of Claim 10, wherein the wavelet transformation comprises a Haar transform.

12. The method of Claim 10, further comprising thresholding the wavelet coefficients of the transformed data block $\tilde{\mathbf{D}}_i$.

13. The method of Claim 10, further comprising applying an inverse wavelet transform to the transformed concentration matrix $\tilde{\mathbf{C}}$ at step i) to provide the concentration matrix **C**.

14. The method of Claim 10, further comprising projecting the product of **T** and **P** onto the spectral shapes matrix **S** from step i) to provide the concentration matrix **C**, according to $\min_{\mathbf{C}} \left\| \mathbf{T}\mathbf{P}^{\mathrm{T}} - \mathbf{C}\mathbf{S}^{\mathrm{T}} \right\|_{\mathbf{F}}$.

15. A method for analyzing multivariate images, comprising:

a) providing a data matrix **D** containing measured spectral data,

b) reading an $i^{th}$ block of data $\mathbf{D}_i$ of a total of $j$ data blocks from the data matrix **D** into the memory of a computer,

c) computing a block crossproduct matrix $\mathbf{D}_i\mathbf{D}_i^T$ from the data block $\mathbf{D}_i$,

d) adding the block crossproduct matrix $\mathbf{D}_i\mathbf{D}_i^T$ to an accumulation of the block crossproduct matrices,

e) repeating steps b) through d) until all $j$ of the data blocks $\mathbf{D}_i$ of the data matrix **D** are read, providing a crossproduct matrix $\mathbf{DD}^T$,

f) performing an eigenanalysis of the crossproduct matrix to obtain eigenvectors **V** and eigenvalues **E**,

g) computing a scores matrix **T**, according to $\mathbf{T} = \mathbf{V}$,

h) computing a loadings matrix **P**, according to $\mathbf{P}^T = \mathbf{T}^T\mathbf{D}$, and

i) performing an image analysis of $\mathbf{TP}^T$ to obtain a concentration matrix **C** and a spectral shapes matrix **S**.

16. The method of Claim 15, wherein the data block $\mathbf{D}_i$ is suitably sized to fit in the memory and consists of the full image planes at some number of spectral channels.

17. The method of Claim 15, wherein $j = 1$.

18. The method of Claim 15, further comprising computing a weighted crossproduct matrix in step e) and using the weighted crossproduct to perform the eigenanalysis in step f).

19. The method of Claim 15, further comprising computing a covariance matrix in step e) and using the covariance matrix to perform the eigenanalysis in step f).

20. The method of Claim 15, further comprising computing a correlation matrix in step e) and using the correlation matrix to perform the eigenanalysis in step f).

21. The method of Claim 15, wherein step f) further comprises retaining only the first *r* columns of **V** so that **T** comprises the first *r* significant eigenvectors of the eigenanalysis.

22. The method of Claim 15, wherein the image analysis comprises an alternating least squares analysis and the concentration matrix **C** and the spectral shapes matrix **S** are obtained from a constrained least squares solution to $\min_{\mathbf{C},\mathbf{S}} \left\| \mathbf{T}\mathbf{P}^{T} - \mathbf{C}\,\mathbf{S}^{T} \right\|_{F}$.

23. The method of Claim 22, wherein the alternating least squares analysis comprises a non-negativity constraint.

24. The method of Claim 15, further comprising applying a wavelet transformation to the data block $\mathbf{D}_i$ after step b), to provide a transformed data block $\tilde{\mathbf{D}}_i$, and using the transformed data block to compute the block crossproduct matrix in step c), to provide a compressed concentration matrix $\tilde{\mathbf{C}}$ at step i).

25. The method of Claim 24, wherein the wavelet transformation comprises a Haar transform.

26. The method of Claim 24, further comprising thresholding the wavelet coefficients of the transformed data block $\tilde{\mathbf{D}}_i$.

27. The method of Claim 24, further comprising applying an inverse wavelet transform to the transformed concentration matrix $\tilde{\mathbf{C}}$ at step i) to provide the concentration matrix **C**.

28. The method of Claim 24, further comprising projecting the product of the **T** and **P** onto the spectral shapes matrix **S** from step i) to provide the concentration matrix **C**, according to $\min_{\mathbf{C}} \left\| \mathbf{T}\mathbf{P}^{T} - \mathbf{C}\mathbf{S}^{T} \right\|_{F}$.

29. A method for analyzing multivariate images, comprising:

a) providing a data factor matrix **A** and a data factor matrix **B** obtained from a factorization of measured spectral data,

b) computing a crossproduct data factor matrix $\mathbf{A}^T\mathbf{A}$ from the data factor matrix **A**,

c) computing a crossproduct data factor matrix $\mathbf{B}^T\mathbf{B}$ from the data factor matrix **B**,

d) performing an eigenanalysis of the product matrix of the crossproduct data factor matrix $\mathbf{A}^T\mathbf{A}$ and the crossproduct data factor matrix $\mathbf{B}^T\mathbf{B}$ to obtain generalized eigenvectors **Y** and eigenvalues **E**,

e) computing a ranked loading matrix $\tilde{\mathbf{P}}$, according to $\tilde{\mathbf{P}} = \mathbf{B}\mathbf{Y}_r$, where $\mathbf{Y}_r$ is the matrix whose columns are the first $r$ columns of **Y**, and

f) computing a ranked scores matrix $\tilde{\mathbf{T}}$, according to $\tilde{\mathbf{T}} = \mathbf{A}(\mathbf{B}^T\mathbf{B})\mathbf{Y}_r$.

30. The method of Claim 29, wherein the factor data matrix **A** comprises $j$ blocks of data factors $\mathbf{A}_i$ and the crossproduct data factor matrix $\mathbf{A}^T\mathbf{A}$ is computed blockwise.

31. The method of Claim 29, wherein the data factor matrix **B** comprises $k$ blocks of data factors $\mathbf{B}_i$ and the crossproduct data factor matrix $\mathbf{B}^T\mathbf{B}$ is computed blockwise.

32. The method of Claim 29, further comprising computing a weighted product matrix at step d) and using the weighted product matrix to perform the eigenanalysis.

33. The method of Claim 29, further comprising computing a covariance matrix at step d) and using the covariance matrix to perform the eigenanalysis.

34. The method of Claim 29, further comprising computing a correlation matrix at step d) and using the correlation matrix to perform the eigenanalysis.

35. The method of Claim 29, further comprising performing an image analysis of $\tilde{\mathbf{T}}\tilde{\mathbf{P}}^T$ to obtain a concentration matrix **C** and a spectral shapes matrix **S**.

36. The method of Claim 35, wherein the image analysis comprises an alternating least squares analysis and the concentration matrix **C** and the spectral shapes matrix **S** are obtained from a constrained least squares solution to $\min_{\mathbf{C},\mathbf{S}} \left\| \tilde{\mathbf{T}}\tilde{\mathbf{P}}^{T} - \mathbf{C}\mathbf{S}^{T} \right\|_{F}$.

37. The method of Claim 36, wherein the alternating least squares analysis comprises a non-negativity constraint.

38. The method of Claim 29, further comprising applying a wavelet transformation to the data factor matrix **A** after step a), to provide a transformed data factor matrix $\tilde{\mathbf{A}}$, and using a transformed data factor matrix $\tilde{\mathbf{A}}^{T}\tilde{\mathbf{A}}$ to compute the crossproduct data factor matrix $\tilde{\mathbf{A}}^{T}\tilde{\mathbf{A}}$ in step b), to provide a transformed scores matrix $\tilde{\tilde{\mathbf{T}}}$ at step f).

39. The method of Claim 38, wherein the wavelet transformation comprises a Haar transform.

40. The method of Claim 38, further comprising thresholding the wavelet coefficients of the transformed data factor matrix $\tilde{\mathbf{A}}$.

41. The method of Claim 38, further comprising performing an image analysis of $\tilde{\tilde{\mathbf{T}}}\tilde{\mathbf{P}}^{T}$ to obtain a transformed concentration matrix $\tilde{\mathbf{C}}$ and a spectral shapes matrix **S**.

42. The method of Claim 41, wherein the image analysis comprises an alternating least squares analysis and the transformed concentration matrix $\tilde{\mathbf{C}}$ and the spectral shapes matrix **S** are obtained from a constrained least squares solution to $\min_{\tilde{\mathbf{C}},\mathbf{S}} \left\| \tilde{\tilde{\mathbf{T}}}\tilde{\mathbf{P}}^{T} - \tilde{\mathbf{C}}\mathbf{S}^{T} \right\|_{F}$.

43. The method of Claim 41, further comprising applying an inverse wavelet transform to the transformed concentration matrix $\tilde{\mathbf{C}}$ to provide a concentration matrix **C**.

44. The method of Claim 41, further comprising projecting the product of the data factor matrix **A** and the data factor matrix **B** from step a) onto the spectral shapes matrix **S** to provide a concentration matrix **C**, according to

$$\min_{\mathbf{C}} \left\| \mathbf{A}\mathbf{B}^{T} - \mathbf{C}\mathbf{S}^{T} \right\|_{F}.$$